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Mechanical Properties of Melt-Quenched MOF Glasses and Their Relation to Microstructure – Will the Neutron Scattering be the Key Tool?

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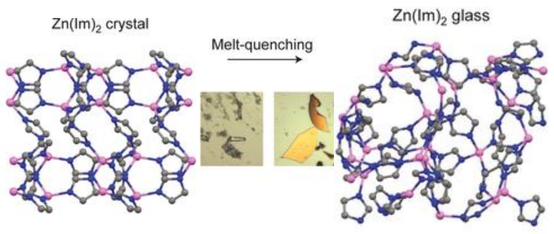
Introduction

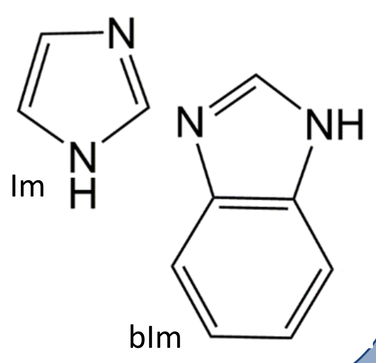


- Metal-organic frameworks are hybrid materials composed of inorganic nodes and organic linkers.
- One of the subsets: ZIF (**Zeolitic Imidazolate Frameworks**).
- It was recently shown that it is possible to vitrify some ZIF crystalline materials by heating up over T_m and rapid cooling [1-3].

How does chemical composition affect properties of MOF glasses?

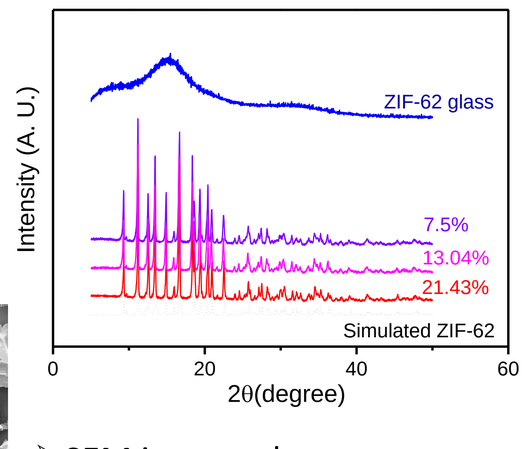
We focus on ZIF-62: zinc nodes connected with two different types of ligands: imidazole (Im, $C_3H_4N_2$) and benzimidazole (bIm, $C_7H_6N_2$).

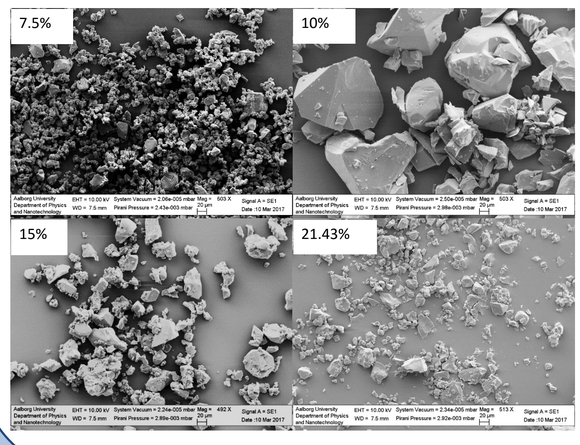
By changing the ratio of ligands during synthesis we study how they influence properties of obtained material.



Synthesis of crystalline ZIF-62 with changing ligand ratio

- Synthesized crystals contained from 7.5% to around 21.5% benzimidazole.
- Powder XRD was preformed in order to ascertain all obtained crystals were ZIF-62.

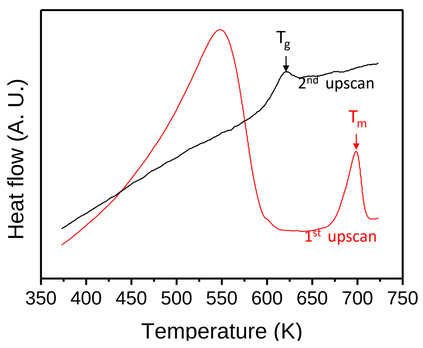




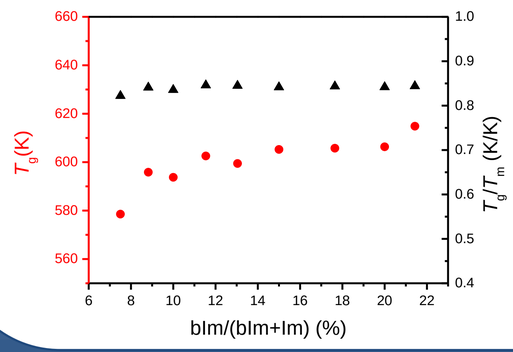
- SEM images show most crystals are of similar size, but those containing 10% bIm – characterized by much larger crystal size.

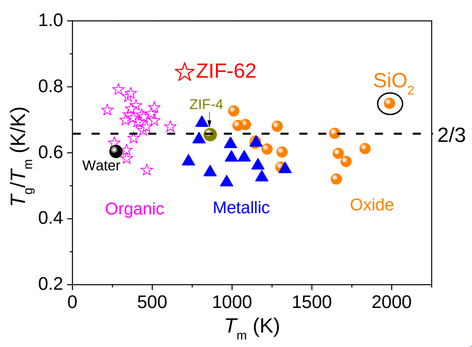
Vitrification and thermal response

- Second upscan shows glass transition peak, Indicating ZIF-62 is vitrified.
- Glass transition temperature (T_g) increases with increasing benzimidazole.



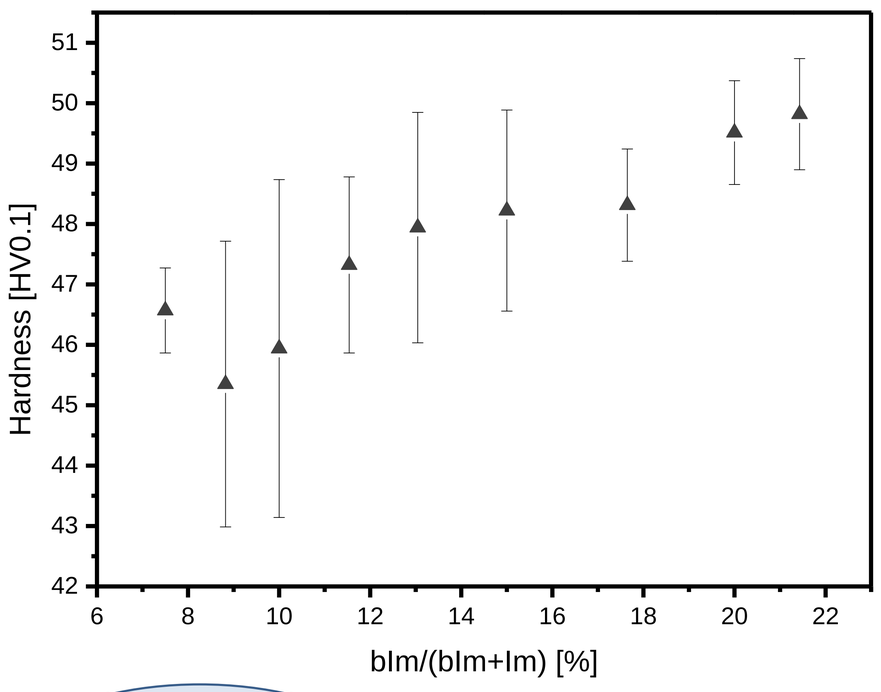
- T_g/T_m is high compared to most glassy materials.





Mechanical properties

An increase of hardness is visible when increasing benzimidazole content:



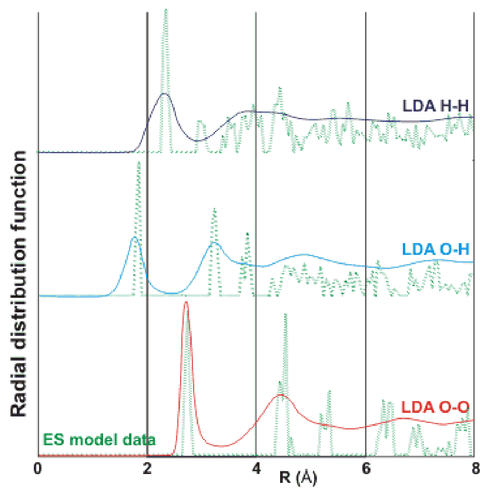
Uncertainty is relatively high – needs to further confirm by additional tests.

Possible source of the error:
- Chemical inhomogeneity;
- Porosity;
- Processing;
- Instrument accuracy.

Why neutron scattering?

To gain deeper insight into structure-properties relations.

- The technique is sensitive for detecting the response of the structure to change of chemical composition, temperature, time...
- It is extremely important for us to characterize the light atoms in organic ligands.



Source: [4]

Conclusion

- Changing the ratio between two different organic ligands influences mechanical properties of ZIF-62 glass.
- The next step is to understand the structural changes. We need sensitive measure – such as neutron scattering.

References

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